

HOW MALTOSE BINDING PROTEINS RECOGNIZE SUBSTRATES: INSIGHTS FROM COMPUTER SIMULATIONS

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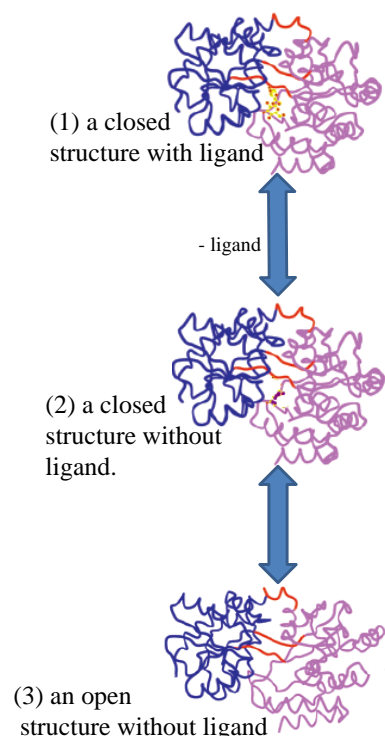


Figure 1. Structural correlation

As a periplasmic component of the Maltose transporter system, the Maltose binding protein (MBP) is known to be able to capture the substrate with high affinity and load it to the entrance of the transmembrane portion of the transporter to initiate the ATP facilitated substrate transportation. Such substrate recognition and binding events trigger a large conformational change in MBP, as suggested from several X-ray crystal structures that capture MBP in an “open” or a “closed” state. To characterize the dynamical natures of these conformational states, we performed Molecular Dynamics (MD) simulations of MBP under three conditions: (1) a closed structure with ligand, (2) a closed structure without ligand, and (3) an open structure without ligand. Based on these equilibrium simulations and additional transition pathway simulations using Targeted Molecular Dynamics (TMD), possible reaction coordinates to describe the conformational change of MBP will be identified. Finally, free energy profiles of the conformational transition will be obtained by umbrella sampling simulations and the molecular recognition mechanism of MBP will be discussed.

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